PATENT SYR-CatS-5002-C1

WE CLAIM:

1. A composition comprising a protein in crystalline form wherein at least a portion of the protein has at least 90% identity with SEQ. ID No. 1.

- 2. A composition according to claim 1 wherein at least a portion of the protein has at least 95% identity with SEQ. ID No. 1.
- 3. A composition according to claim 1 wherein at least a portion of the protein comprises consecutively of SEQ. ID No. 1.
- 4. A composition according to claim 1 wherein the protein crystal diffracts X-rays for a determination of structure coordinates to a resolution greater than 3.0 Angstroms.
- 5. A composition according to claim 1 wherein the protein crystal has a crystal lattice in a P4₁22 space group.
- 6. A composition according to claim 1 wherein the protein crystal has a crystal lattice having unit cell dimensions, +/- 5%, of a=b= 85.159Å and c=152.18Å.
- 7. A composition comprising CatS in crystalline form wherein the crystal has a crystal lattice in a $P4_122$ space group.
- 8. A composition comprising CatS in crystalline form wherein the crystal has a crystal lattice having unit cell dimensions, +/- 5%, of a=b= 85.159Å and c=152.18Å.
- 9. A method for forming a crystal of a protein comprising:

forming a crystallization volume comprising: a precipitant solution and a protein wherein at least a portion of the protein has at least 90% identity with SEQ. ID No. 1; and

storing the crystallization volume under conditions suitable for crystal formation of the protein.

10. A method according to claim 9 wherein at least a portion of the protein has at least 95% identity with residues SEQ. ID No. 1.

PATENT SYR-CatS-5002-C1

11. A method according to claim 9 wherein at least a portion of the protein comprises consecutively of SEQ. ID No. 1.

- 12. A method according to claim 9 wherein the protein crystal diffracts X-rays for a determination of structure coordinates to a resolution greater than 3.0 Angstroms.
- 13. A method according to claim 9 wherein the protein crystal has a crystal lattice in a P4₁22 space group.
- 14. A method according to claim 9 wherein the protein crystal has a crystal lattice having unit cell dimensions, +/- 5%, of a=b= 85.159Å and c=152.18Å.
- 15. A method according to claim 9, the method further comprising diffracting the protein crystal to produce a diffraction pattern and solving the structure of the protein from the diffraction pattern.
- 16. A composition comprising an isolated protein consisting of SEQ. ID No. 1.
- 17. A composition according to claim 16 where the protein is expressed from a nucleic acid molecule that comprises SEQ. ID No. 2.
- 18. A composition comprising an isolated protein consisting of SEQ. ID No. 3.
- 19. A method of identifying an entity that associates with a protein comprising: taking structure coordinates from diffraction data obtained from a crystal of a protein that has at least 90% identity with SEQ. ID No. 3; and

performing rational drug design using a three dimensional structure that is based on the obtained structure coordinates.

- 20. A method according to claim 19 wherein the protein has at least 95% identity with SEQ. ID No. 3.
- 21. A method according to claim 19 wherein the protein crystal has a crystal lattice having unit cell dimensions, +/- 5%, of a=b= 85.159Å and c=152.18Å.

PATENT SYR-CatS-5002-C1

22. A method according to claim 19 wherein the protein crystal has a crystal lattice in a P4₁22 space group.

- 23. A method according to claim 19, the method further comprising selecting one or more entities based on the rational drug design and contacting the selected entities with the protein.
- 24. A method according to claim 19, the method further comprising measuring an activity of the protein when contacted with the one or more entities.
- 25. A method according to claim 19, the method further comprising comparing activity of the protein in a presence of and in the absence of the one or more entities; and selecting entities where activity of the protein changes depending whether a particular entity is present.
- 26. A method according to claim 19, the method further comprising contacting cells expressing the protein with the one or more entities and detecting a change in a phenotype of the cells when a particular entity is present.